MATHEMATICAL MODELS RELATING EFFECTS OF XENOBIOTIC SUBSTANCES ON INDIVIDUALS AND POPULATIONS

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LONG TERM GOALS

The research involves the development of mathematical models suitable for relating the effects of xenobiotic substances on individuals and populations of benthic marine organisms. This goal recognizes that the ecological effects of contaminants occur within complex ecological communities, but that the response of the constituent populations to environmental stress is difficult and/or very expensive to measure. Thus it is important to extract as much insight as possible from the large body of experimental information quantifying the impact of toxicants on the individual organisms within impacted, or potentially impacted populations.

OBJECTIVES

The research has two main parts: (i) modeling the consequences for individuals of toxicant-induced changes in the rates of energy acquisition and utilization by individual organisms, and (ii) using individual-based population models to predict the implications of these changes on the abundance and spatial distribution of organisms.

APPROACH

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Our research makes use of two types of models. In modeling the response of individuals to toxicants, we use dynamic energy budget (DEB) models to describe the rules by which individual organisms assimilate and utilize energy from food. They incorporate feeding and assimilation rates dependent on the state of the individual and the environment, together with rules for energy allocation to maintenance, growth and reproduction (including priorities for energy allocation when food is scarce). Thus DEB models constitute a natural context within which to model the mechanisms whereby vital biological rates (growth, reproduction, respiration) are influenced by exposure to contaminants. In particular, DEB models offer a systematic conceptual framework within which to identify general principles from the large body of information relating to specific toxicants and/or impacted genus, species, or even life stage.

In modeling spatially explicit populations, we use individual-based population models. Individual organisms are distributed over a two-dimensional grid, and interact with each other and with the environment in accordance with rules that are a simplified version of the rules describing individual energetics, supplemented with assumptions on mortality. This approach allows a rigorous implementation of individual behavior and physiology at the population level, and also allows for dynamic change in the spatial distribution of interacting organisms.

WORK COMPLETED

Highlights of FY97 include:

- Formulation and testing of general, DEB-based theory describing reduced growth in early life stages of marine organisms due to sublethal contaminant exposure.
- Demonstration of our ability to use energetic considerations to predict the outcome of competition among marine snails.
- Completion of a study contrasting the predictions of individual-based population models with predictions from traditional models.

RESULTS

DEB-based theory of toxicant action

Our models of toxicant action are based on the theory of Kooijman (1993), which has recently been extensively used to interpret standardized toxicity tests (Kooijman and Bedaux 1996 and references therein). We assume that toxicants change the energy fluxes by affecting the model parameters. A DEB model has three kinds of parameters: rates, efficiencies and a constant characterizing the partitioning of assimilated food between somatic and reproductive tissue. In the sublethal range, toxicants have been shown to have a smaller effect on efficiencies than on rates, and rate parameters are thus assumed to be the primary targets of toxicant action. These assumptions allow us to describe the effects of a wide range of metallic and lipophillic toxicants, but exclude consideration of environmental estrogens.

The plausibility of some of the model assumptions was confirmed using data on suborganismal processes. We then tested the model’s fit to literature data on growth, covering a wide variety of animals and toxicants. The systems tested were, in increasing order of complexity: mitochondrial respiration with cadmium and two lipophilic

compounds, 2,4,6-trichlorophenol (TCP) and 2,4-dinitrophenol (DNP); feeding and respiration by the mussel *Mytilus edulis* in the presence of toluene or pentachlorophenol; larval growth of the oyster *Crassostrea gigas* and the mussel *M. galloprovencialis* reared at different mercury concentrations; the growth of the earthworm *Lumbricus rubellus* in soils contaminated with copper; and the growth of the zebrafish *Brachydanio rerio* in the presence of a polycyclic aromatic hydrocarbon (PAH) or a mixture of PAHs. In all cases, the model gave satisfactory descriptions of the data. Details are in Muller and Nisbet (submitted).

Energy utilization and competition among marine snails

Traditional competition theory assumes closed populations, and thus has limited relevance to local marine populations. Yet understanding of local, short-term population dynamics is an essential prerequisite to predicting the effects of environmental stress. We developed a model for two consumers feeding on a single resource, and tested its predictions using a microalgal-gastropod system in which two coexisting grazers (*Tegula eisini* and *T. aureotincta*) feed on a common resource (Schmitt 1996). *T. eisini* is a “digger”, moving slowly and grazing the algae down to almost bare substrate, whereas *T. aureotincta* is a “grazer”, moving more quickly and leaving behind a larger fraction of the algal layer. These complementary foraging strategies structure the algal resource. We estimated model parameters using data from Schmitt's experimental studies of *Tegula*. The model revealed that foraging complementarity leads to changes in resource structure that that likely facilitates coexistence. Details are in Wilson et al. (submitted).

Comparison of individual-based and traditional population models

Throughout this project, we have used individual-based models. One long-standing puzzle is that these models make predictions on the stability and spatial distribution of populations, that differ fundamentally from those generated using the reaction diffusion formalism that is popular in oceanography. We have identified the cause of these differences, and have thereby achieved conceptual unification of two diverse theoretical methods. The key difference is that *local* stochastic effects, subsumed into the diffusion term of most reaction-diffusion models may significantly change the dynamics. Understanding this allows us to introduce new parameters into the reaction-diffusion model, and then reproduce the individual-based simulation results. This simplification opens the possibility of making the individual-to-population transition over much larger spatial scales. Details are in Wilson (in press).

IMPACT

Each of the papers described above represent significant advances in the field. There is already considerable conceptual unification at the chemical end of ecotoxicology (for example through quantitative structural-activity relationships (QSARs). Our work, taken with that of Kooijman and Bedaux (1996), represents the first attempt to develop similarly general theory that will allow a single model framework to encompass a diverse range of organisms. The study of competition among snails takes a very original approach, and opens the possibility of using energetic-based models to relate the outcome of competition to environmental change. The comparison of individual-based and

population models not only resolves a long-standing issue in ecological theory, but brings our population modeling much closer to the mainstream effort in oceanography.

TRANSITIONS

The research is not yet at a point to move from research into the Navy fleet or to industry. It has been used in a project related to off-shore oil production (see below).

RELATED PROJECTS

- The work on dynamics energy budget modeling has proceeded in parallel with a project, funded by the Southern California Educational Initiative of the Minerals Management Service, which involved modeling the effects of produced water on growth and reproduction of mussels. In particular, Dr. E.B. Muller, a post-doctoral researcher employed with that support, has made valuable contributions to the present work.
- We have met with Dr. K. Carman to discuss using our modeling approach in interpreting data form his studies of benthic microcosms.

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